



# **Urban Scale Aerosol Dispersion Modeling**

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**Adaptive Urban Dispersion Modeling**

**April 15, 2004**

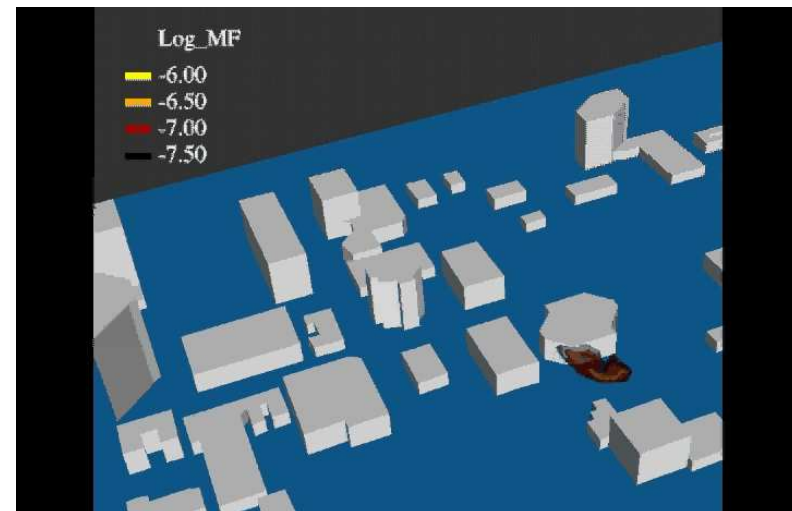
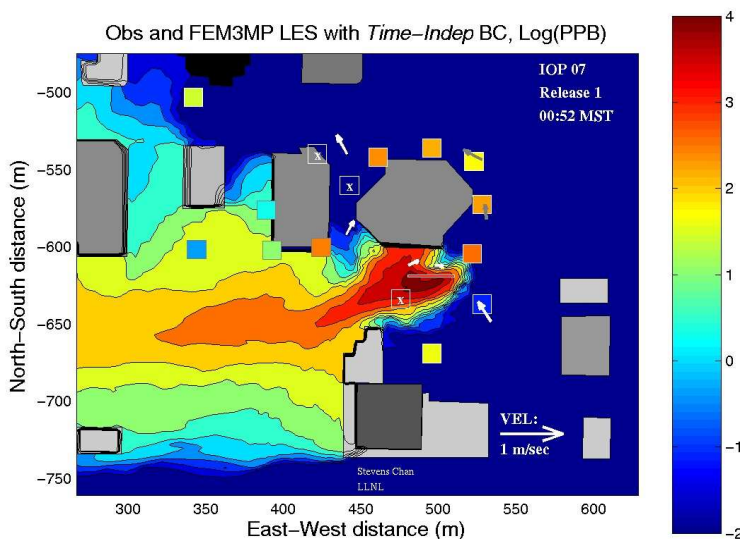




# Prediction of aerosol dispersion is a critical homeland security need



- High fidelity models that predict the spread of airborne hazardous materials are important
  - Field experiments are difficult and expensive
  - Assist in emergency planning and response scenarios
  - Guide effective sensor placement
  - Event reconstruction (with measurements)

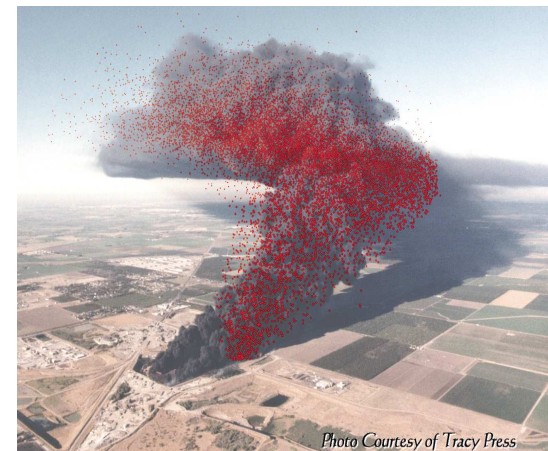




# NARAC: An operational release advisory center at LLNL



- **National Atmospheric Release Advisory Center**
  - Supports the DHS Emergency Preparedness and Response (EPR) directorate
  - Provides detailed predictions of atmospheric releases for real-time emergency response, pre-planning, and post-incident assessments
  - Incorporates hierarchy of models for different types of release events, distance scales, and response times

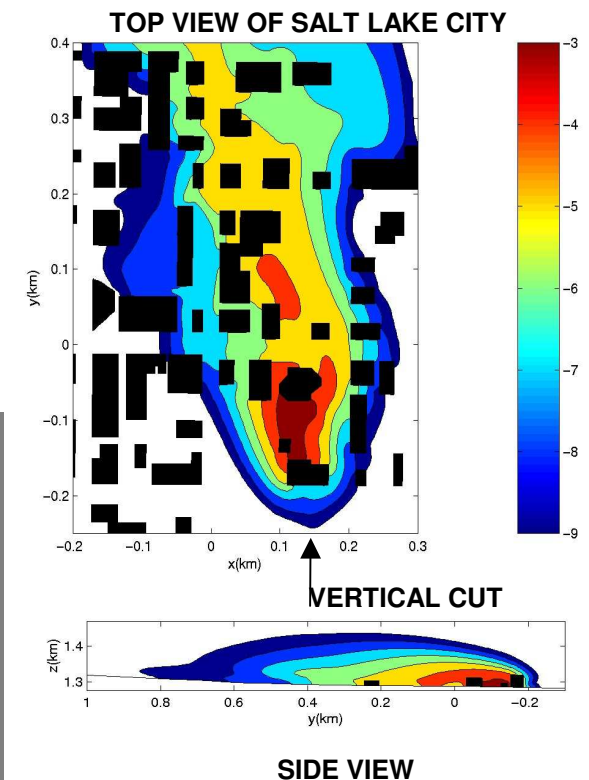
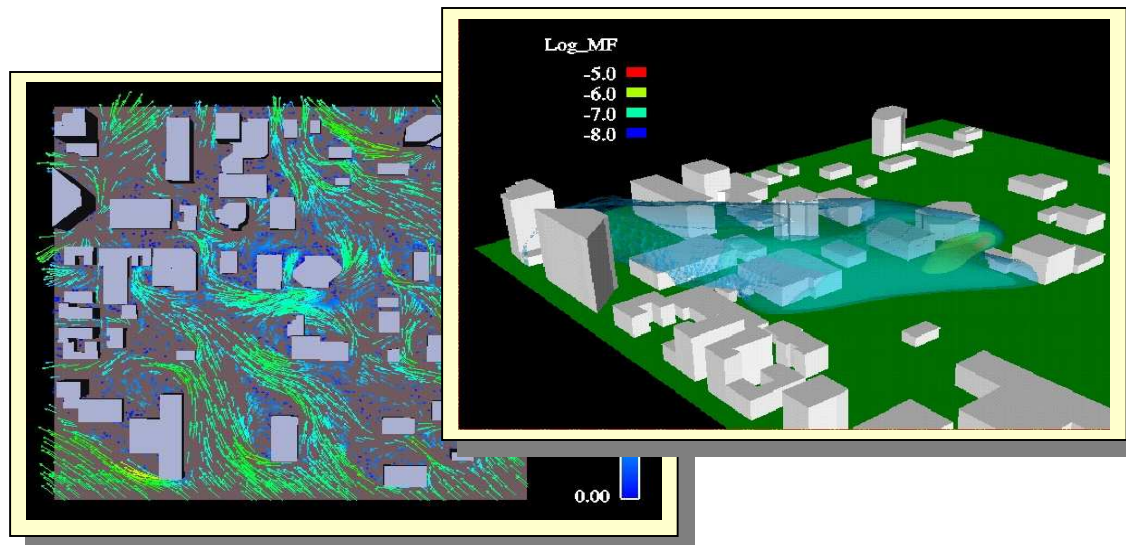




# NARAC has models for urban dispersion simulation



- **FEM3MP is the primary urban dispersion modeling code used in the atmospheric sciences division in NARAC**
  - Finite element incompressible CFD
  - Structured mesh
  - LES & RANS turbulence models
  - Atmospheric chemistry



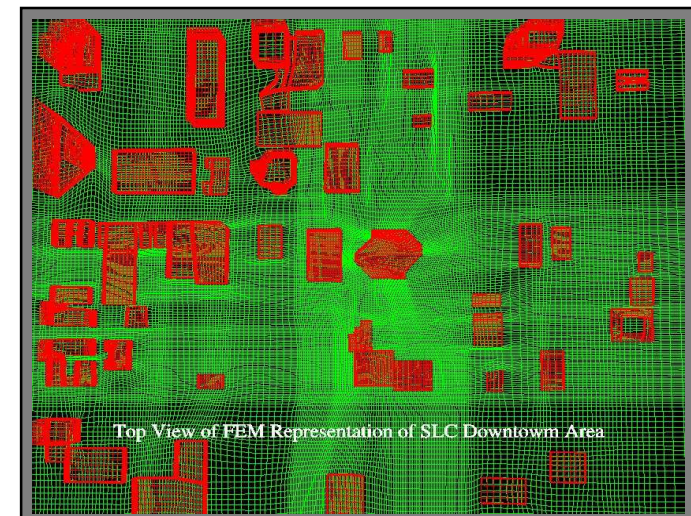
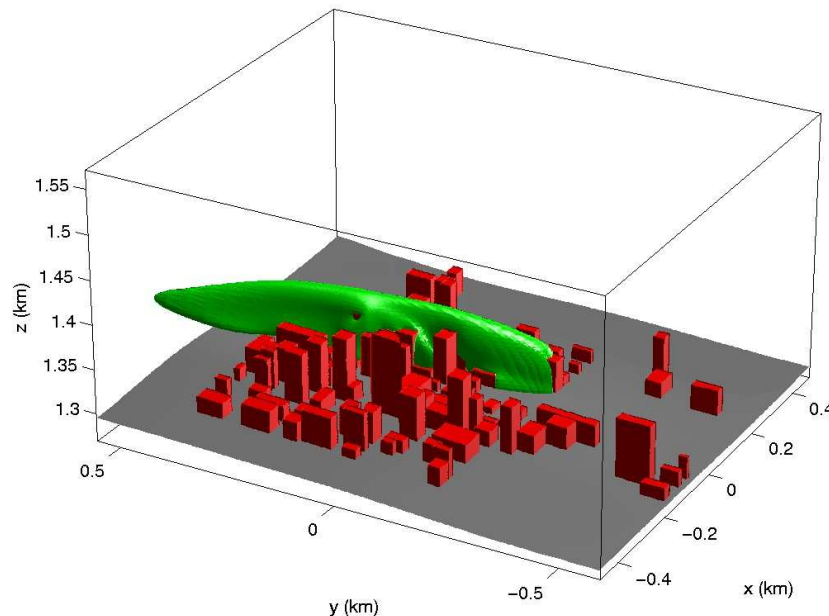




# Current urban modeling capability has some limitations



- Unable to resolve complex building geometries
- Labor-intensive grid generation
- Limited capability for fast evolving flows
- Limited range of release scenarios (e.g., moving sources)

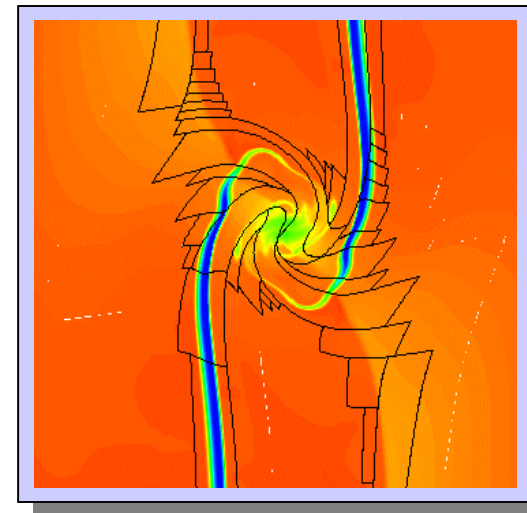
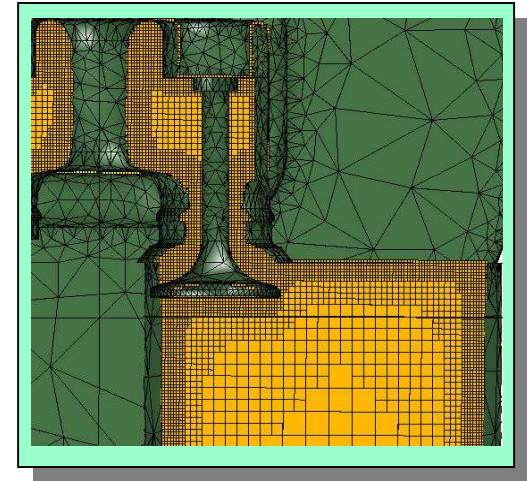




# We are developing advanced meshing tools to enhance capabilities

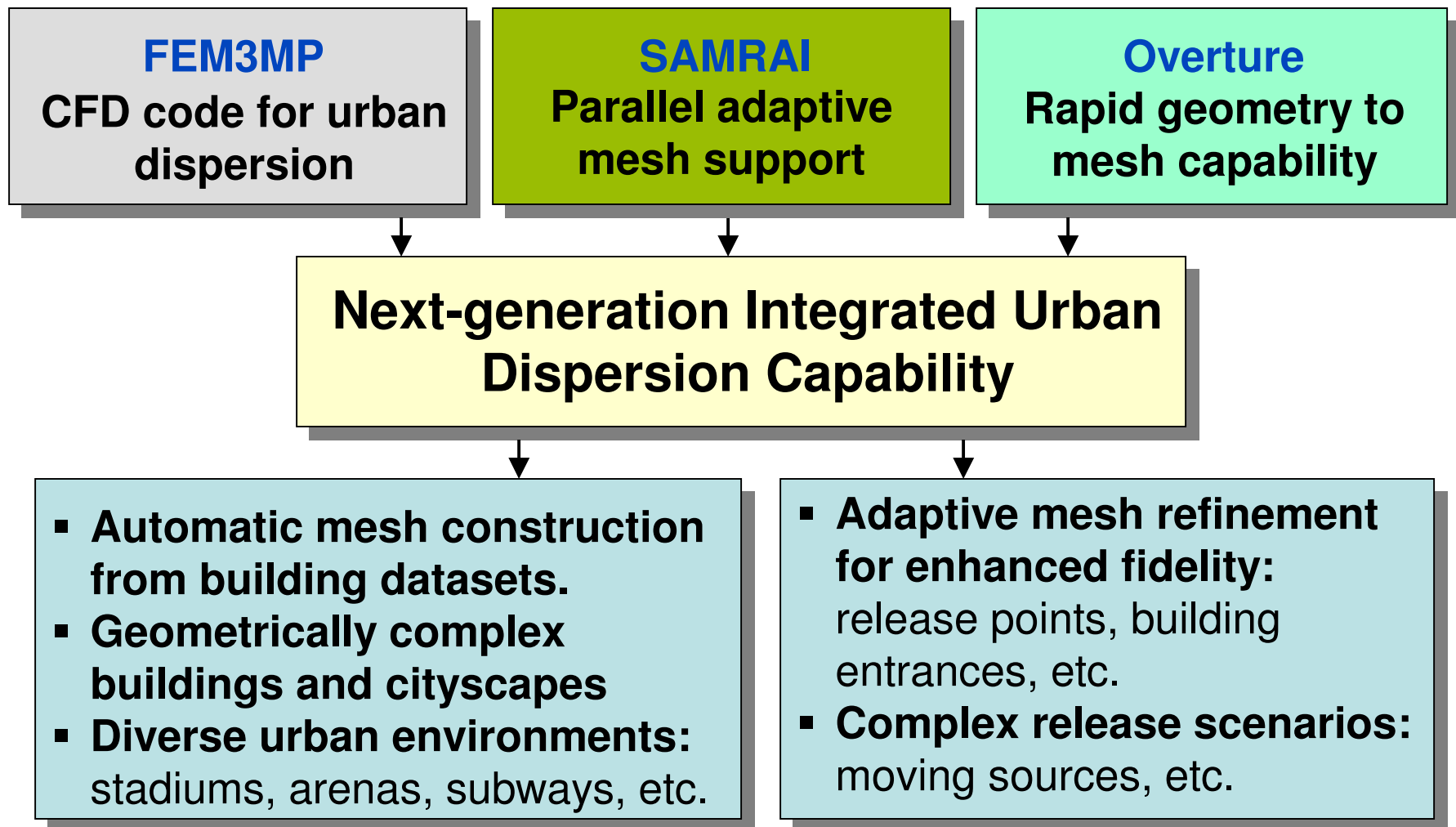


- **Overture** project has tools for rapid geometry-to-mesh (Rapsodi)
  - Rapid construction of surface grids from CAD data
  - Interfaces to fast volume grid generator from NASA (CUBES)
- **SAMRAI** infrastructure supports parallel AMR applications
  - Data structures for flexible mesh geometry
  - Adaptive mesh refinement
  - Scalability verified on  $> 1K$  processors



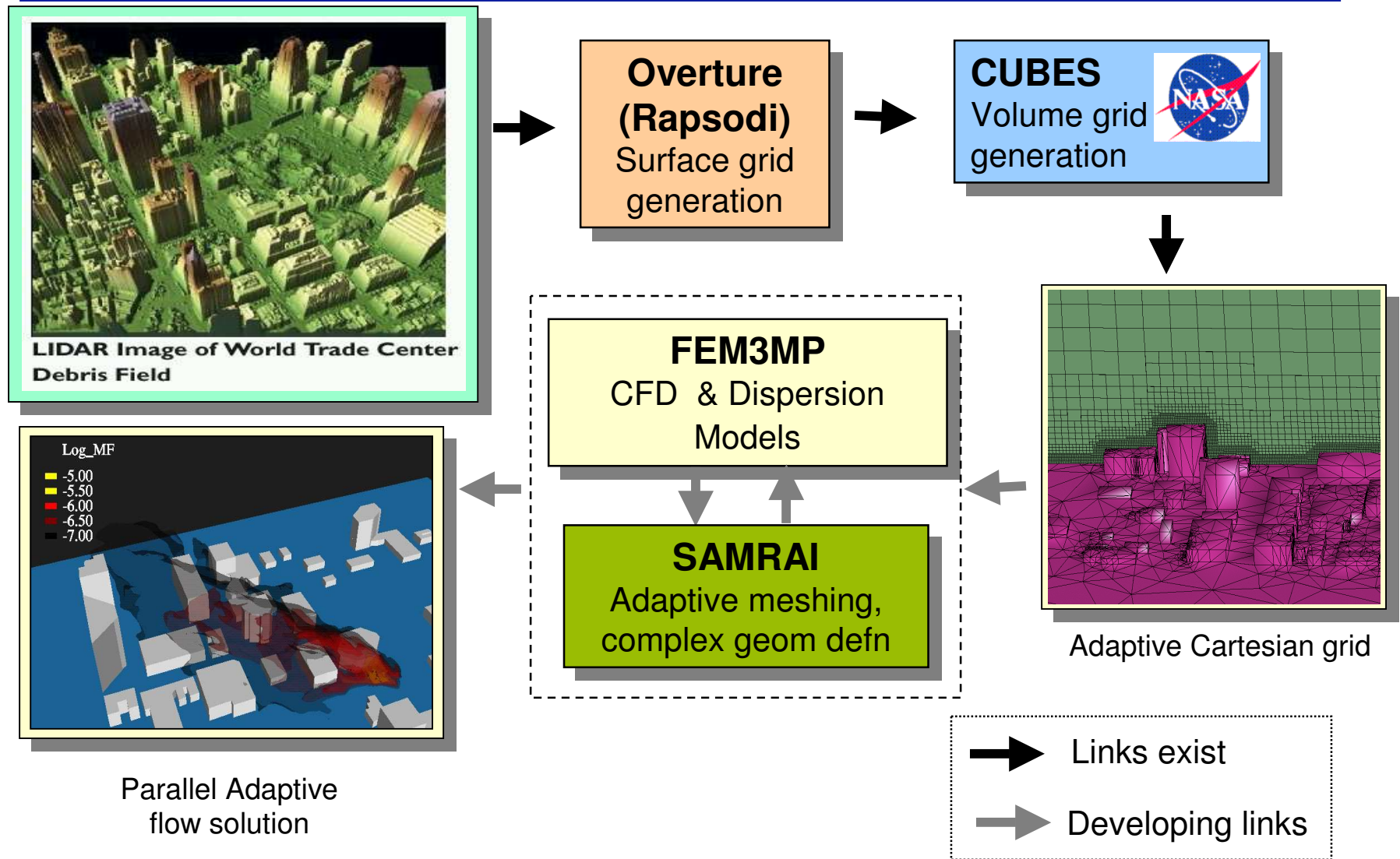


# Couple technologies to develop an operational tool





# Integrated approach will enable automated geometry to CFD analysis



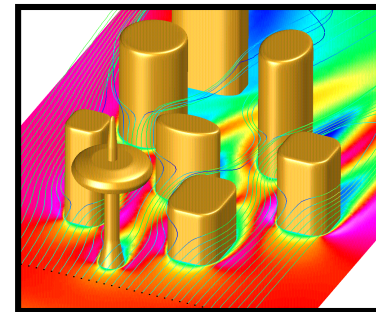
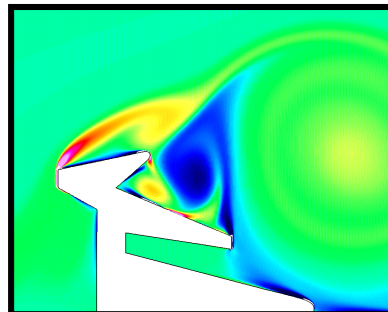
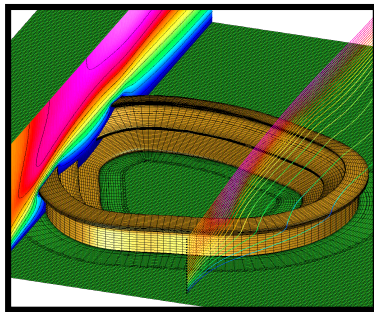




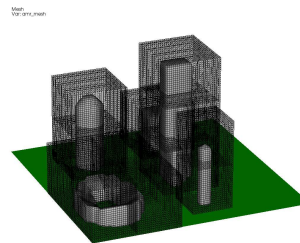
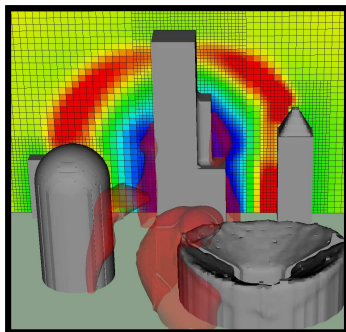
# Some demonstration calculations around complex building geometries



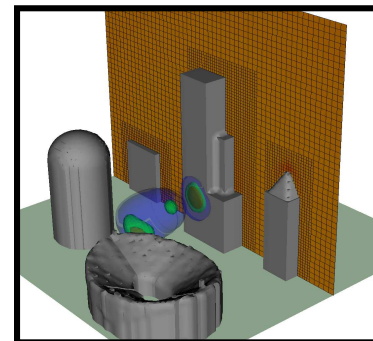
- Flow around stadium and sample cityscape with overset grids



- Adaptive flow simulation over prototype cityscape with cut-cell grids

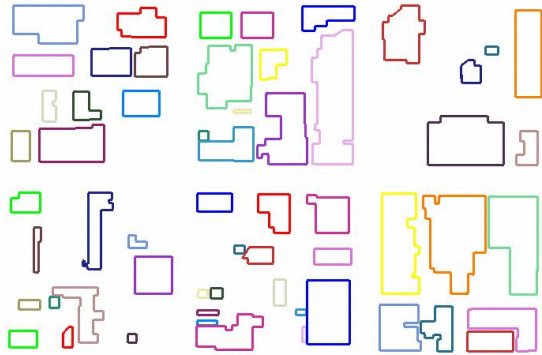


Refined region  
around buildings

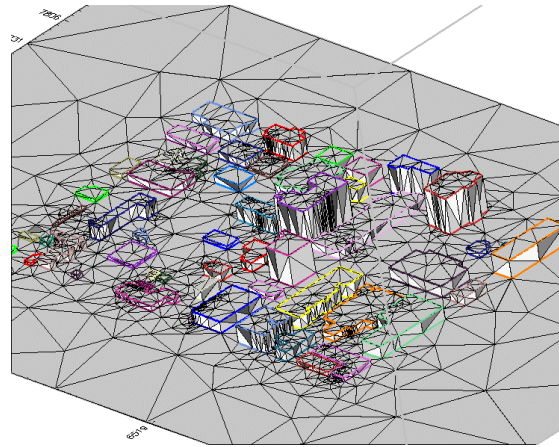




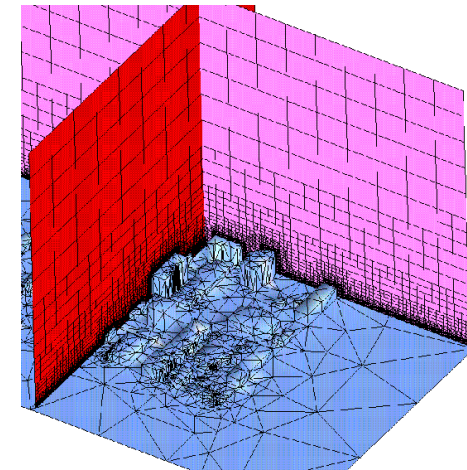
# Automatic construction of grids from building datasets



**Polygonal  
geometry data  
(Salt Lake City)**



**Surface triangulation  
by **metro****



**AMR volume  
mesh by **CUBES****

- “metro” reads building geometry data and generates surface triangulation and CUBES input
- Prof. Marsha Berger, NYU Courant, is a CUBES co-developer and a collaborator on this project

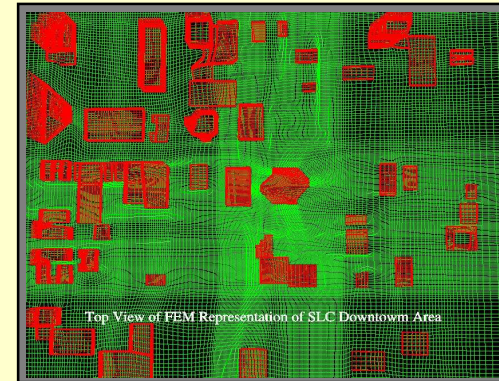


# Grid generation time reduced from weeks to minutes



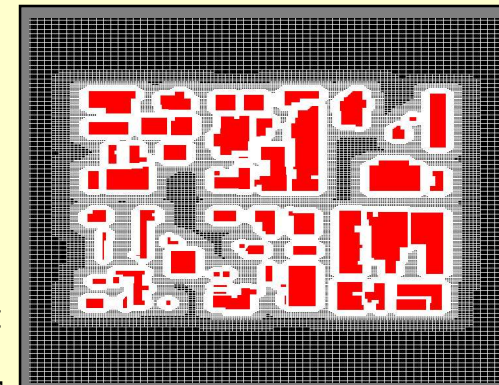
## Downtown Salt Lake City gridding example

- Structured grid constructed with existing tools required about 1 week



- Adaptive cut-cell grid generated with metro + CUBES required about 2 minutes

1.7M gridpoints, 6 levels refinement  
Surface grid – 30 sec with “metro”  
Volume grid – 45 sec with “CUBES”

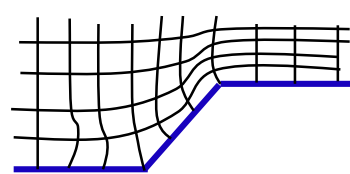




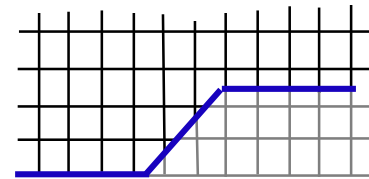
# Research Issues to be addressed in 2004-2005



- Finite element boundary representation on cut-cell grids using “fictitious domain” algorithm



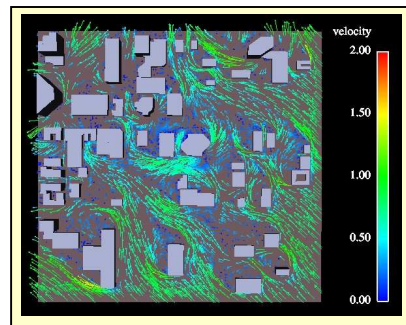
“conforming” mesh (old)



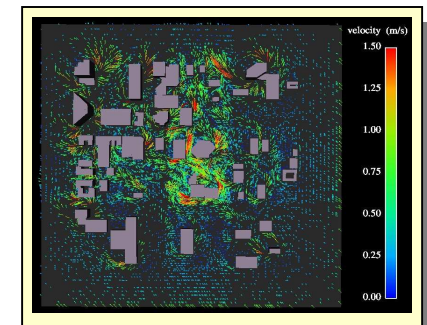
“cut-cell” mesh (new)

- Adaptive algorithms for finite element CFD solver
- Turbulence models

RANS



LES



- Building geometry information that incorporates new features (e.g. terrain)



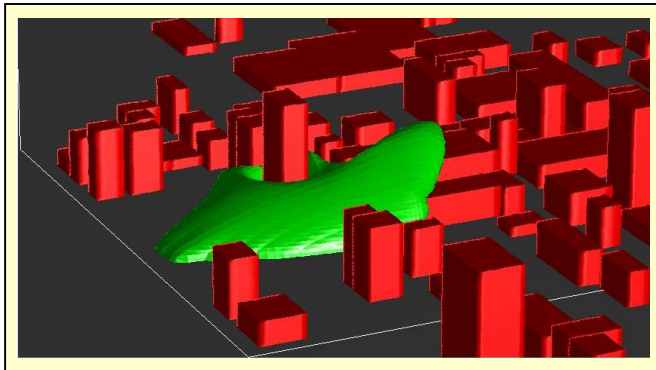
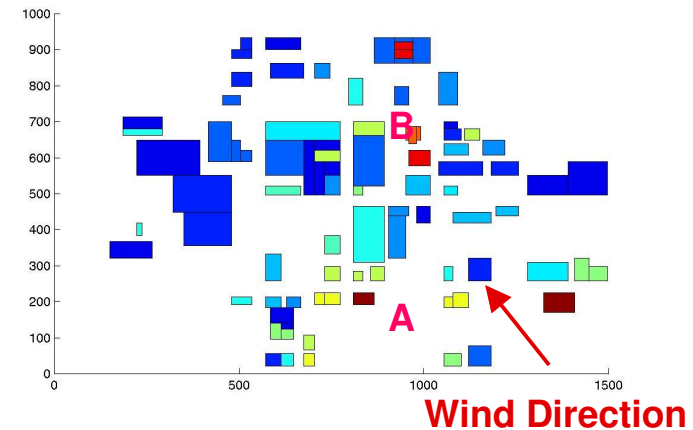


# We will use experimental data to verify and validate model accuracy

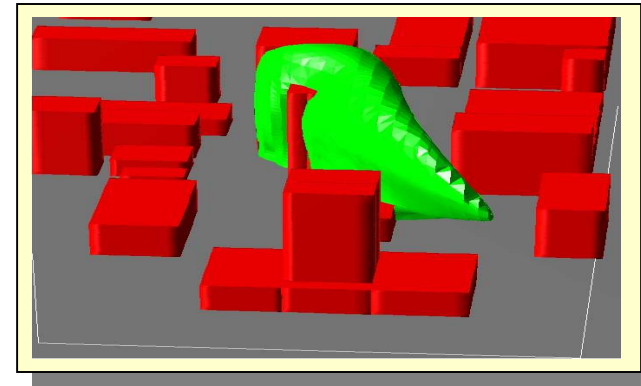


- Joint-Urban 2003 in Oklahoma City
- Urban 2000 in Salt Lake City
- Wind tunnel experiments

## Downtown Oklahoma City



Release south of downtown (A)



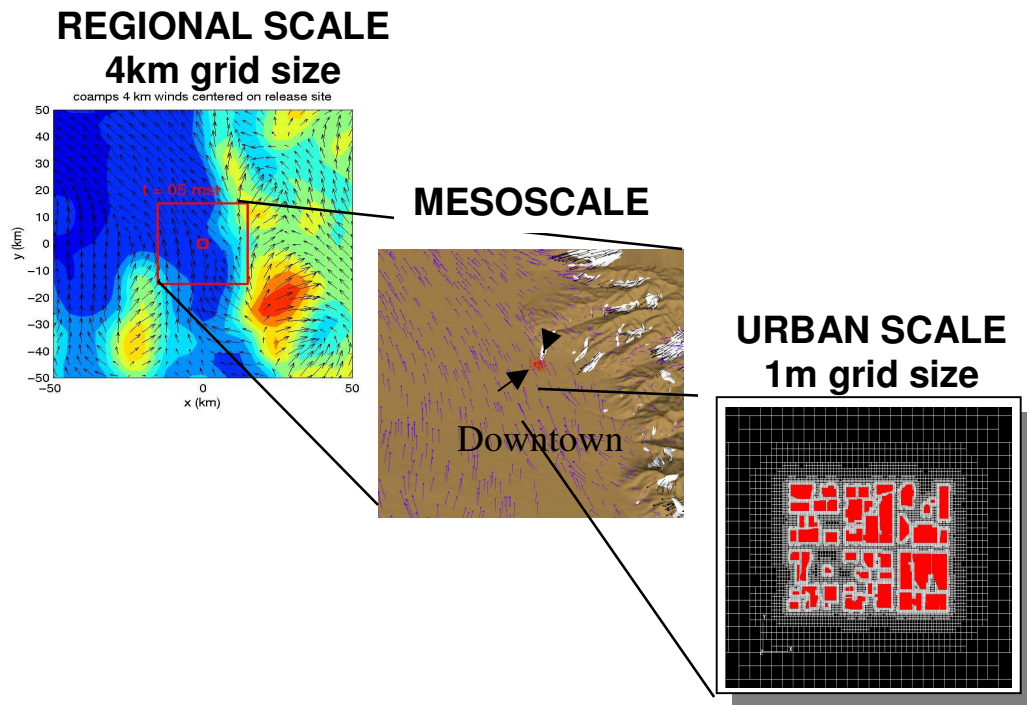
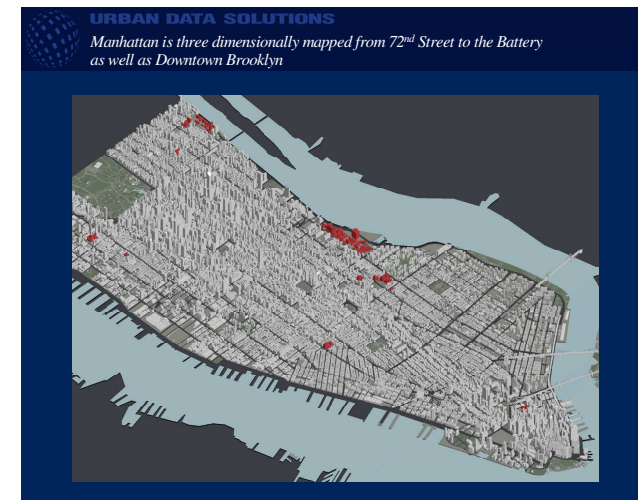
Release in downtown area (B)



# Longer term research issues



- Coupling models with different scales
- Integrate our external model with internal flow models (subways, arenas, etc.) – J. Shadid, SNL



- Large-scale cityscapes (e.g. Manhattan)
- Performance on diverse parallel architectures



# A next-generation airborne dispersion modeling capability



- We are pursuing a new urban dispersion modeling tool by combining technologies developed in CASC and NARAC
- Fast problem setup and adaptive gridding capabilities will make the tool a candidate for inclusion in NARAC's operational set of models
- Anticipate tool with primary features will be ready by late 2005

